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A Monte Carlo Approach to Calculate Probability Tables for the Unresolved-Resonance Region Using the AMPX Cross-Section Processing System

M. E. Dunn

Oak Ridge National Laboratory,*
P. O. Box 2008,
Oak Ridge, TN 37831-6370 USA
(865) 574-5260

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In neutron cross-section evaluations, energy-averaged unresolved-resonance parameters are typically provided for the unresolved-resonance region (URR). Due to the statistical nature of the unresolved-resonance parameters, probability tables can be used to provide cross-section probability distribution functions for energy ranges at specific temperatures within the URR. Different approaches can be used to generate probability tables for an isotope of interest. The historical approach is to generate continuous-energy cross-section data from a "ladder" of resonances and determine contributions to a probability table based on the point data. A new and different procedure relative to the "ladder" approach is used in the AMPX cross-section processing system. A new module, PURM (**P**robability tables for the **U**nresolved **R**egion using **M**onte Carlo), has been developed for AMPX.

PURM uses a Monte Carlo approach to calculate probability tables on an evaluator-defined energy grid in the URR. For each probability table, PURM samples a Wigner spacing distribution for pairs of resonances surrounding the reference energy. The resonance distribution is sampled for each spin sequence (i.e., ℓ, J pair), and PURM uses the Δ_3-statistics test to determine the number of resonances to sample for each spin sequence. For each resonance, PURM samples the resonance widths from a Chi-square (χ^2) distribution for a specified number of degrees of freedom. Once the resonance parameters are sampled, PURM calculates the total, capture, fission and scatter cross sections at the reference energy using the single-level Breit-Wigner formalism with appropriate treatment for temperature effects. The cross-section calculation constitutes a single iteration or history. For the cross-section calculation and corresponding probability-table calculation, PURM processes a user-specified number of batches with a corresponding number of histories per batch. For each history, PURM calculates the total, capture, fission and scatter cross section at the reference energy, and the corresponding contribution to the probability table is determined for each history. After completing the specified number of histories for a batch, a batch estimate for the probability for each cross-section band within a table is obtained by dividing the number of tallies for the band by the total number of histories processed. Additional batches are processed until the user-specified number of batches are complete. Due to the nature of the calculational procedures, PURM provides a mechanism for monitoring the convergence of the cross-section calculation. For each reaction, a plot of the calculated cross section is provided by batches run. Additional statistical checks are provided for each cross-section calculation.

In an effort to establish the capabilities of PURM, probability tables have been calculated for the ^{235}U (ENDF/B-VI) URR. The PURM-generated probability tables for ^{235}U were compared with probability tables generated using the NJOY module PURR. The probability tables and cross-section values that were calculated by PURM and NJOY are in agreement, and the verification studies with NJOY establish the computational capability for generating probability tables using the new AMPX module PURM.